```
=> d his

     (FILE 'HOME' ENTERED AT 14:00:48 ON 09 AUG 2001)

     FILE 'REGISTRY' ENTERED AT 14:00:52 ON 09 AUG 2001
L1             STRUCTURE UPLOADED
L2              13 S L1
L3             199 S L2 FULL

     FILE 'CA' ENTERED AT 14:01:31 ON 09 AUG 2001
L4              24 S L3
L5              13 S L4 AND PD < JULY 1999
L6               1 S L5 AND BJORSNE, M?/AU
L7              12 S L5 NOT L6

     FILE 'CAOLD' ENTERED AT 14:03:24 ON 09 AUG 2001
L8               3 S L3

     FILE 'REGISTRY' ENTERED AT 14:03:44 ON 09 AUG 2001
                E   7038-02-0/RN
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STRUCTURE FILE UPDATES: 10 AUG 2001 HIGHEST RN 351153-64-5
DICTIONARY FILE UPDATES: 10 AUG 2001 HIGHEST RN 351153-64-5

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> e bispidine/cn

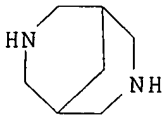
```
E1            1     BISPHOSPHOLO(1,2-A:2',1'-C)(1,4)DIPHOSPHORIN, TUNGSTEN
DERIV
                    ./CN
E2            1     BISPIDIN/CN
E3            1 --> BISPIDINE/CN
E4            1     BISPIDINEBENZAMIDE/CN
E5            1     BISPIDINOL/CN
E6            1     BISPRASIN/CN
E7            1     BISPROMAZINE/CN
E8            1     BISPROPARGYL SULFIDE/CN
E9            1     BISPROPOXUR SULFIDE/CN
E10           1     BISPROPYLIDENEANILINE/CN
E11           1     BISPUUPEHENONE/CN
E12           1
BISPYRANO(2'',3'':5',6')PYRANO(2',3':5,6)PYRANO(3,2-B:2',3'-
                    F)OXEPIN/CN
```

=> s e3

L1 1 BISPIDINE/CN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
RN 280-74-0 REGISTRY
CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Bispidin
CN **Bispidine**
FS 3D CONCORD
MF C7 H14 N2
CI COM, RPS
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, GMELIN*, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



16 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
17 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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Trying 3106016892...Open

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LOGINID:ssspta1612BXR
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


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 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2  Dec 17   The CA Lexicon available in the CAPLUS and CA files
 NEWS  3  Feb 06   Engineering Information Encompass files have new names
 NEWS  4  Feb 16   TOXLINE no longer being updated
 NEWS  5  Apr 23   Search Derwent WPINDEX by chemical structure
 NEWS  6  Apr 23   PRE-1967 REFERENCES NOW SEARCHABLE IN CAPLUS AND CA
 NEWS  7  May 07   DGENE Reload
 NEWS  8  Jun 20   Published patent applications (A1) are now in USPATFULL
 NEWS  9  JUL 13   New SDI alert frequency now available in Derwent's
                   DWPI and DPCI

 NEWS EXPRESS  July 11 CURRENT WINDOWS VERSION IS V6.0b,
               CURRENT MACINTOSH VERSION IS V5.0C (ENG) AND V5.0JB (JP),
               AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2001
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 14:00:48 ON 09 AUG 2001

=> file reg

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.15       0.15

FILE 'REGISTRY' ENTERED AT 14:00:52 ON 09 AUG 2001
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STRUCTURE FILE UPDATES: 8 AUG 2001 HIGHEST RN 350791-61-6
DICTIONARY FILE UPDATES: 8 AUG 2001 HIGHEST RN 350791-61-6

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

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L1 STRUCTURE UPLOADED

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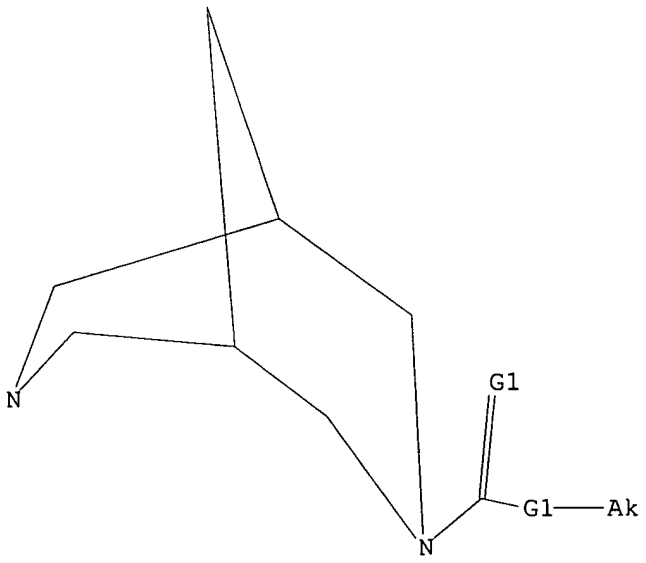
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:01:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 46 TO ITERATE

100.0% PROCESSED 46 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 514 TO 1326
PROJECTED ANSWERS: 44 TO 476

L2 13 SEA SSS SAM L1

=> s l2 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 14:01:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 884 TO ITERATE

100.0% PROCESSED 884 ITERATIONS 199 ANSWERS
SEARCH TIME: 00.00.01

L3 199 SEA SSS FUL L1

=> file ca

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	133.56	133.71

FILE 'CA' ENTERED AT 14:01:31 ON 09 AUG 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1947 - 2 Aug 2001 VOL 135 ISS 7
FILE LAST UPDATED: 2 Aug 2001 (20010802/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

The CA file now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

The CA Lexicon is now available in the Controlled Term (/CT) field.

Enter HELP LEXICON for full details.


```
=> s l3

L4          24 L3

=> s l4 and pd < july 1999

      17796360 PD < JULY 1999
                 (PD<19990700)
L5          13 L4 AND PD < JULY 1999

=> s l5 and bjorsne, m?/au

             4 BJORSNE, M?/AU
L6           1 L5 AND BJORSNE, M?/AU

=> d l6, ibib abs fhitstr, 1


L6   ANSWER 1 OF 1  CA  COPYRIGHT 2001 ACS
ACCESSION NUMBER:        131:58860  CA
TITLE:                   Preparation of 3,7-diazabicyclo[3.3.1]nonane-3-
                         carboxylates as antiarrhythmic agents
INVENTOR(S):             Strandlund, Gert; Alstermark, Christer; Bjore,
Annika;
                       Bjorsne, Magnus; Frantsi, Marianne;
                         Halvarsson, Torbjorn; Hoffmann, Kurt-Jurgen;
                         Lindstedt, Eva-Lotte; Polla, Magnus
PATENT ASSIGNEE(S):      Astra Aktiebolag, Swed.
SOURCE:                  PCT Int. Appl., 129 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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     WO 9931100         A1   19990624       WO 1998-SE2276    19981210 <--
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             DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
             KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
             MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
             TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     ZA 9811130         A    19990617       ZA 1998-11130     19981204 <--
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AU 9917953	A1	19990705	AU 1999-17953	19981210
BR 9813668	A	20001017	BR 1998-13668	19981210
EP 1047695	A1	20001102	EP 1998-962796	19981210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
NO 2000003137	A	20000817	NO 2000-3137	20000616

PRIORITY APPLN. INFO.: SE 1997-4709 A 19971217
WO 1998-SE2276 W 19981210

OTHER SOURCE(S): MARPAT 131:58860

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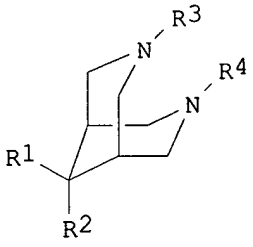


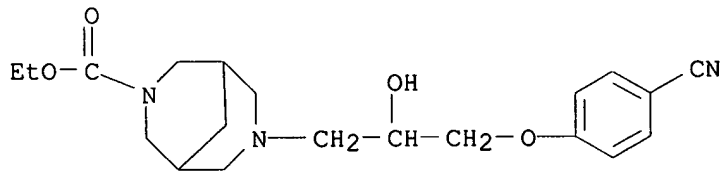
I

AB Title compds. [I; R1,R2 = H or alkyl; R1R2 = OCH2CH2O, (CH2)4-5; R3 = CCR10R11AR; A = bond, alkylene, (CH2)nZ, CONR20, etc.; B = bond, alkylene, NR23(CH2)r, O(CH2)r; R = (un)substituted Ph; R4 = COXR9; R9 = alkyl, (un)substituted phenyl(alkyl), -naphthyl; R10 = H or OH; R11,R20,R23 = H or alkyl; X = O or S; Z = NR20, SO0-2, O; n,r = 0-4] were prepd. Thus, 4-(NC)C6H4OH was condensed with epichlorohydrin and the product aminated by I (R1 = R2 = H, R4 = CO2CMe3)(II; R3 = H)(prepn. given) to give II [R3 = CH2CH(OH)CH2OC6H4(CN)-4]. Data for biol. activity of I were given.

IT **227939-98-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3,7-diazabicyclo[3.3.1]nonane-3-carboxylates as antiarrhythmic agents)

RN 227939-98-2 CA

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3
REFERENCE(S): (1) Basf Aktiengesellschaft; EP 0308843 A2 1989 CA

(2) Kall-Chemie Pharma Gmbh; EP 0306871 A2 1989 CA
(3) The Board Of Regents Of Oklahoma State University;
WO 9107405 A1 1991 CA

=> d his

(FILE 'HOME' ENTERED AT 14:00:48 ON 09 AUG 2001)

FILE 'REGISTRY' ENTERED AT 14:00:52 ON 09 AUG 2001
L1 STRUCTURE UPLOADED
L2 13 S L1
L3 199 S L2 FULL

FILE 'CA' ENTERED AT 14:01:31 ON 09 AUG 2001
L4 24 S L3
L5 13 S L4 AND PD < JULY 1999
L6 1 S L5 AND BJORSNE, M?/AU

=> s l5 not l6

L7 12 L5 NOT L6

=> d l7, ibib abs fhitstr, 1-12

L7 ANSWER 1 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 132:12427 CA
TITLE: An efficient chemoenzymatic access to chiral 3,7-diazabicyclo[3.3.1]nonane derivatives
AUTHOR(S): Danieli, Bruno; Lesma, Giordano; Passarella, Daniele; Silvani, Alessandra; Viviani, Nunzia
CORPORATE SOURCE: Dipartimento di Chimica Organica e Industriale, Universita degli Studi di Milano, Centro CNR di Studio per le Sostanze Organiche Naturali, Milan, 21-20133, Italy
SOURCE: Tetrahedron (**1999**), 55(40), 11871-11878
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
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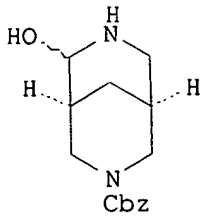

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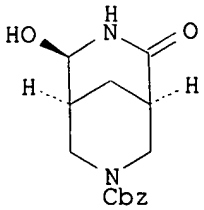


II

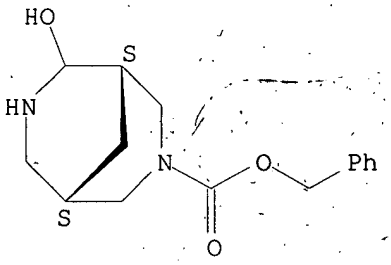
AB Enantiopure 3,7-diazabicyclo[3.3.1]nonane derivs. I and II, potential precursors of quinolizidine alkaloids, were synthesized in high yields, starting from the biocatalytic asymmetrization of .sigma.-sym. 3,5-disubstituted piperidines. Their application to the total synthesis of the new pharmacol. active compds. are also described.

IT **251346-88-0P**
RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(chemoenzymic access to chiral 3,7-diazabicyclo[3.3.1]nonane derivs.)

RN 251346-88-0 CA

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 6-hydroxy-, phenylmethyl ester, (1S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17

REFERENCE(S):
(3) Danieli, B; J Org Chem 1998, V63, P3492 CA
(4) Danieli, B; Tetrahedron 1994, V50, P8837 CA
(5) Danieli, B; Tetrahedron: Asymm 1996, V7, P345 CA
(6) Dess, D; J Am Chem Soc 1991, V113, P7277 CA
(7) Fazylov, S; Zh Obshch Khim 1995, V65, P877 CA
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 12 CA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 128:180115 CA

TITLE: Stereochemistry of N-acetyl-r-2,c-4-diphenyl-3-azabicyclo[3.3.1]nonanes and N-ethoxycarbonyl-r-2,c-4-diphenyl-3-azabicyclo[3.3.1]nonane

AUTHOR(S): Jeyaraman, R.; Ponnuswamy, S.

CORPORATE SOURCE: Department of Chemistry, Bharathidasan University, Tiruchirapalli, 620 024, India

SOURCE: Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem. (**1997**), 36B(9), 730-737
CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication, CSIR

DOCUMENT TYPE: Journal

LANGUAGE: English

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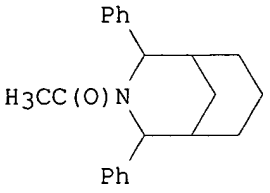

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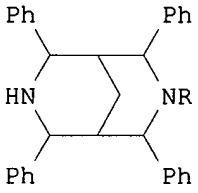


II

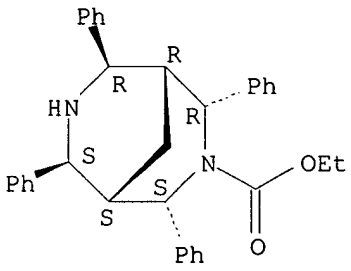
AB The conformational preferences of N-acetyl-r-2,c-4-diphenyl-3-azabicyclo[3.3.1] nonane I and N-ethoxycarbonyl-and N-acetyl-r-2,c-4,t-6,t-8-tetraphenyl-3,7-diazabicyclo[3.3.1] nonanes II (R= CO2Et,COMe) have been studied using NMR spectral techniques. The azabicyclo[3.3.1]nonane I is found to prefer a twin-chair conformation with a slight flattening at the nitrogen end. In the case of diazabicycles II both the ethoxycarbonylation and acetylation reactions are found to take place only at the boat end of the parent amine and the preferred conformation of the products is found to be twin-chair with flattening at C1-C2-N3-C4-C5 part of the ring in both cases. The energy barrier for the N-CO rotation in N-ethoxycarbonyl deriv. 6 has been detd. from the dynamic 1H NMR studies and the barrier for N- CO rotation is found to be 50.8 kJ mol-1, much less than that of N-nitroso analogs.

IT **203190-52-7P**, N-(Ethoxycarbonyl)-r-2,c-4-diphenyl-3-azabicyclo[3.3.1]nonane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(dynamic NMR conformational anal. of ethoxycarbonyl-and acetyltetraphenyldiazabicyclononanes)

RN 203190-52-7 CA

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2,4,6,8-tetraphenyl-, ethyl ester, (2R,4S,6S,8R)-rel-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 3 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 126:8107 CA
TITLE: Preparation of diazabicyclo(3.3.1)nonane derivatives

for the treatment of Alzheimer's disease and cerebral function disorders

INVENTOR(S): Kobayashi, Koji; Orita, Kazuhiro; Hamada, Atsushi; Inaba, Takashi; Abe, Hiroyuki; Miyazaki, Susumu

PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan

SOURCE: PCT Int. Appl., 128 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9630372	A1	19961003	WO 1996-JP742	19960321 <--
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RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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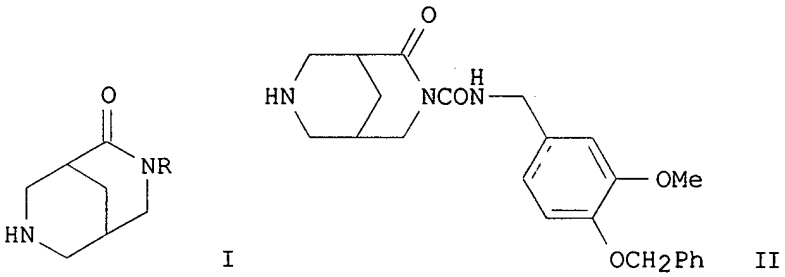
JP 08325267	A2	19961210	JP 1996-66858	19960322 <--

PRIORITY APPLN. INFO.: JP 1995-66497 19950324
WO 1996-JP742 19960321

OTHER SOURCE(S): MARPAT 126:8107

GI



AB The title compds. I [R represents CONH(CHR1)mR2, etc.; R1 represents hydrogen or alkyl; m is 0, 1 or 2; and R2 represents optionally substituted aryl, optionally substituted heterocycle, optionally substituted cycloalkyl, alkyl or alkenyl] are prepd. I have nicotinic cholinergic effect and dopamine-releasing effect. In an in vitro test for affinity for the nicotinic acetylcholine receptors, the title compd. II fumaric acid salt showed IC50 of 57 nM, vs. 25 nM for nicotine.

IT **183277-39-6P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of diazabicyclononane derivs. for treatment of Alzheimer's disease and cerebral function disorders)

RN 183277-39-6 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2-oxo-, phenylmethyl ester, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

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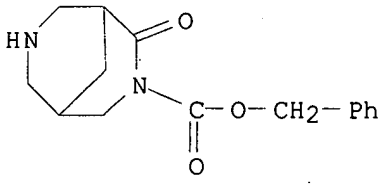
CRN 183277-38-5
CMF C15 H18 N2 O3



CM 2

CRN 110-17-8
CMF C4 H4 O4
CDES 2:E

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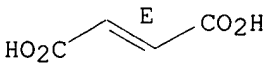
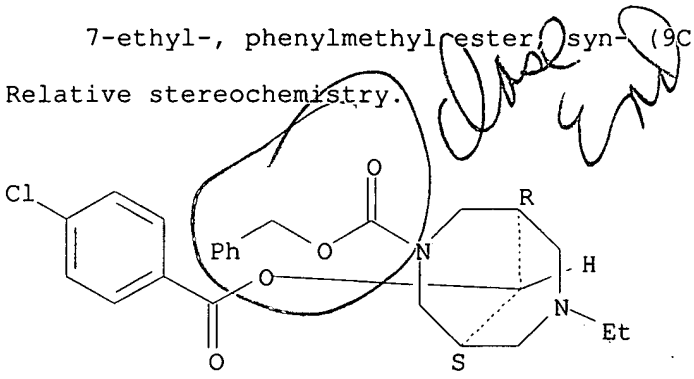


L7 ANSWER 4 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 123:111879 CA
TITLE: Synthesis and biological activity of the metabolites of syn-3-ethyl-7-methyl-3,7-diazabicyclo[3.3.1]non-9-yl 4-chlorobenzoate hydrochloride
AUTHOR(S): Yamawaki, Ichiro; Bukovac, Scott W.; Sunami, Akihiko
CORPORATE SOURCE: Tokushima Res. Cent., Pharmacokinetics Res. Lab. and Pharmacol. Res. Lab., Tokushima, 771-01, Japan
SOURCE: Chem. Pharm. Bull. (**1994**), 42(11), 2365-9
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:111879
AB Five metabolites of syn-3-ethyl-7-methyl-3,7-diazabicyclo[3.3.1]non-9-yl 4-chlorobenzoate hydrochloride (YUTAC) were prepd. and examd. for Na+ current blocking activity in guinea pig ventricular myocytes. These metabolites showed lower inhibitory activities than the parent compd. or were inactive.
IT **166272-89-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and Na+ current blocking activity of the metabolites of Yutac)
RN 166272-89-5 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-[(4-chlorobenzoyl)oxy]-

7-ethyl-, phenylmethyl ester, syn- (9CI) (CA INDEX NAME)

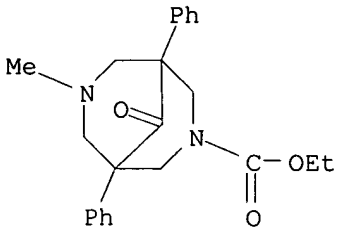
Relative stereochemistry.



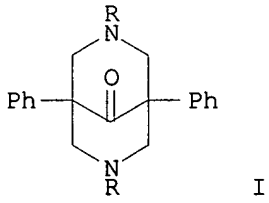
L7 ANSWER 5 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 112:54544 CA
TITLE: Conformations of derivatives of 3,7-diazabicyclo[3.3.1]nonan-9-one. Comparison of 3-ethoxycarbonyl-7-methyl-1,5-diphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one and 3,7-bis(ethoxycarbonyl)-1,5-diphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one: effect of a nucleophile.cntdot..cntdot..cntdot.electrophile interaction on molecular geometry
AUTHOR(S): McCabe, Peter H.; Milne, Neal J.; Sim, George A.
CORPORATE SOURCE: Chem. Dep., Univ. Glasgow, Glasgow, G12 8QQ, UK
SOURCE: J. Chem. Soc., Perkin Trans. 2 (**1989**), (7), 831-4
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English

AB X-ray analyses of 3-ethoxycarbonyl-7-methyl-1,5-diphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one (I) and 3,7-bis(ethoxycarbonyl)-1,5-diphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one (II) have established that both mols. adopt twin-chair conformations. In II, the urethane N atoms have the expected nearly coplanar arrangement of bonds, whereas in I, the urethane N atom has a distinctly pyramidal pattern of bonds; the N-CO2Et bond in I is bent out of the CH2-N-CH2 plane towards the NMe group so that the N...C sepn. between the NMe and CO2Et groups is 2.665 .ANG. whereas the corresponding distances in II are 3.363 and 3.150 .ANG.. The results demonstrate the existence of an attractive nucleophile-electrophile interaction in I.

IT **7037-98-1**
RL: PRP (Properties)
(crystal structure and conformation of)
RN 7037-98-1 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-methyl-9-oxo-1,5-diphenyl-, ethyl ester (7CI, 8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 6 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 103:123460 CA
TITLE: Conformational control in the 3,7-diazabicyclo[3.3.1]nonane system
AUTHOR(S): McCabe, P. H.; Milne, N. J.; Sim, G. A.
CORPORATE SOURCE: Chem. Dep., Univ. Glasgow, Glasgow, G12 8QQ, UK
SOURCE: J. Chem. Soc., Chem. Commun. (**1985**), (10), 625-6
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:123460
GI

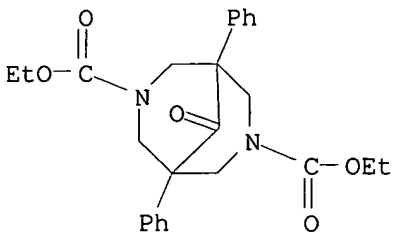


I

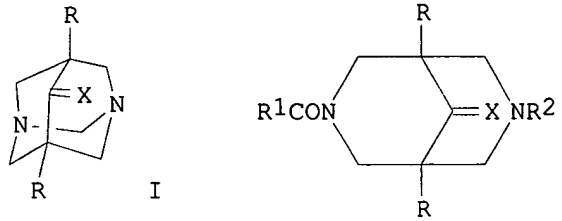
AB Twin-chair or boat-chair conformations of the title system can be selected by forming N,N'-derivs. in which the N atoms have planar or pyramidal bonding patterns, resp. Thus, crystal structure anal. of the diazabicyclononane derivs. I (R = NO, CO2Et, COCF3) showed mols. with essentially planar bonding patterns at N and with twin-chair conformation, whereas a similar study of I (R = SO2C6H4Me-4, Me) showed mols. with boat-chair conformations and a distinctly pyramidal arrangement of bonds at N.

IT **13638-71-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., crystal and mol. structure, and conformation of, substituent effect on)

RN 13638-71-6 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-oxo-1,5-diphenyl-, diethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)

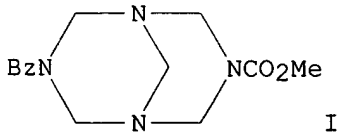


L7 ANSWER 7 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 100:156576 CA
TITLE: Synthesis and transformations of polyhedral compounds.
VII. Ring opening of azaadamantanes by mixed anhydrides
AUTHOR(S): Agadzhanyan, Ts. E.; Arutyunyan, G. L.; Minasyan, G. G.; Movsesyan, R. A.
CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SOURCE: Arm. Khim. Zh. (**1983**), 36(10), 669-72
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

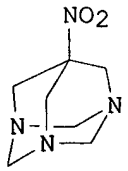


I

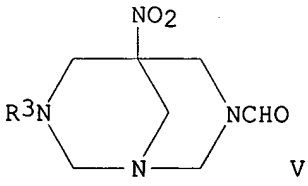
II



III



IV

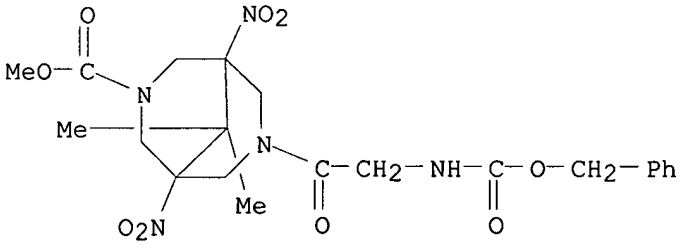


V

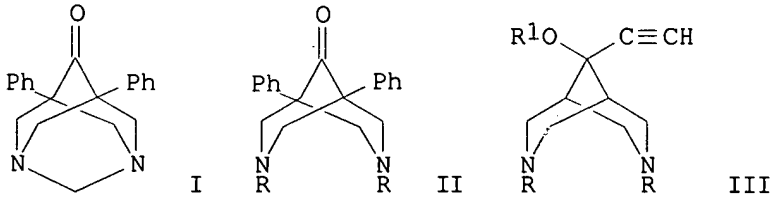
AB Diazaadamantanes I (R = NO2, X = Me2) was treated with R1CO2CO2Me (R1 = PhCH2O2CNHCH2, BzNHCH2) to give diazabicyclononanes II (R2 = CO2Me). Analogously, urotropine and BzOCO2Me gave 40% tetraazabicyclononane III. Treating I (R = Ph, X = O) with HCO2OAc gave 42% II (R = Ph, R1 = H, R2 = CHO). Addnl. obtained from triazaadamantane IV were triazabicyclononanes V (R3 = CHO, Ac).

IT **89250-89-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
RN 89250-89-5 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9,9-dimethyl-1,5-dinitro-7-[[[(phenylmethoxy)carbonyl]amino]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

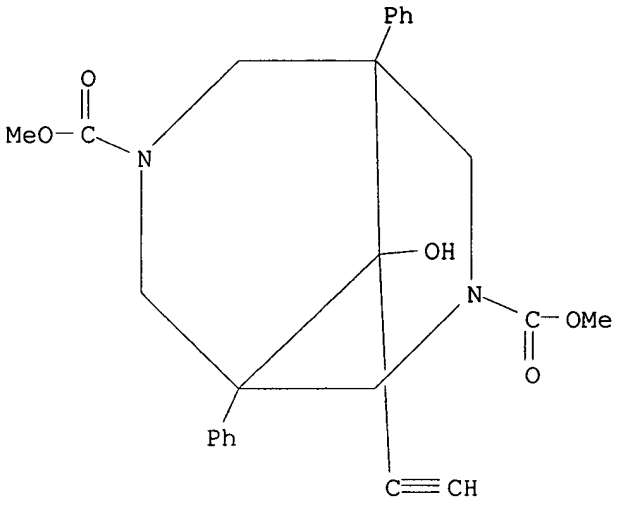


L7 ANSWER 8 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 99:194908 CA
TITLE: Synthesis and stereochemistry of the heteroanalogs of bicyclononane and adamantane. Ethynylation of 1,5-diphenyl-3,7-diacyl-3,7-diazabicyclo[3.3.1]nonanes
AUTHOR(S): Gubasheva, A. Sh.; Omarov, T. T.
CORPORATE SOURCE: Inst. Khim. Nauk, Alma-Ata, USSR
SOURCE: Deposited Doc. (**1982**), VINITI 3358-82, 9 pp. Avail.: VINITI
DOCUMENT TYPE: Report
LANGUAGE: Russian
GI

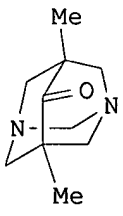


AB Acylation of I by RCOCl (R = Ac, Bz, CO2Me, CO2Et) gave diacyl derivs. II which underwent addn. with HC.tplbond.CH to give III (R1 = H). Esterification of the latter gave III (R1 = Ac, Bz, CO2Me, CO2Et).
IT **87703-23-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)
RN 87703-23-9 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-ethynyl-9-hydroxy-

1,5-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 96:104172 CA
TITLE: Synthesis and reactions of polyhedral compounds. II. Synthesis of 5,7-dimethyl-1,3-diazaadamantan-6-one and
-6-ol and their conversion into 3,7-diacyl(dicarbalkoxy, diarylsulfonyl)-3,7-diazabicyclo[3,3,1]nonanes
AUTHOR(S): Agadzhanyan, Ts. E.; Arutyunyan, G. L.
CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SOURCE: Arm. Khim. Zh. (**1981**), 34(11), 963-8
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



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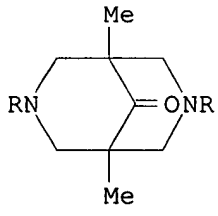
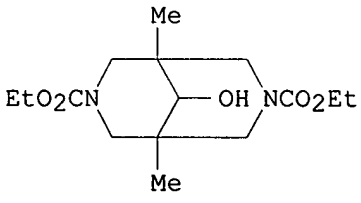


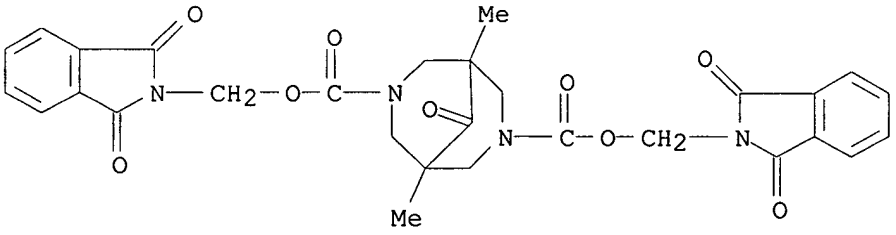
II



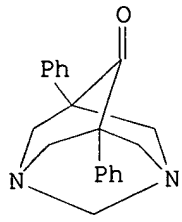
III

AB Cyclocondensation of EtCOEt, HCHO, and AcONH4 gave 19.5% I, which reacted with RCOCl, RO2CCl, or ArSO2Cl to give II [R = BrCH2CO, BrCH2CH2CO, CH2:CHCO, Bz, (phthalimidomethoxy)carbonyl, EtOCO, PhCH2OCO, 4-MeC6H4SO2, 4-(MeO2CNH)C6H4SO2]. LiAlH4 redn. of I gave 83.3% alc., which with ClCO2Et gave III.

IT **80808-91-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 80808-91-9 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 1,5-dimethyl-9-oxo-, bis[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl] ester (9CI) (CA INDEX NAME)



L7 ANSWER 10 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 95:132841 CA
TITLE: Synthetic conversions in a series of bicyclo[3.3.1]nonane and adamantane diaza analogs
AUTHOR(S): Gubasheva, A. Sh.
CORPORATE SOURCE: USSR
SOURCE: Vestn. Akad. Nauk Kaz. SSR (**1981**), (4), 66-7
CODEN: VANKAM; ISSN: 0002-3213
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



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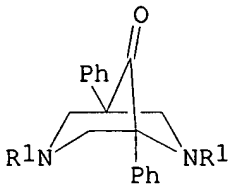
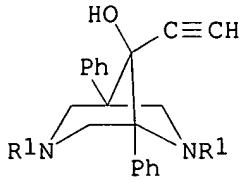
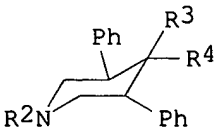


II



III

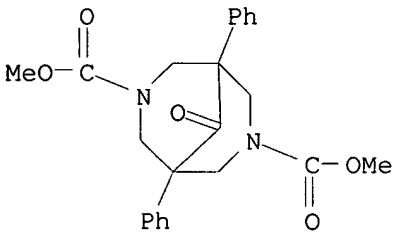


IV

AB Diazaadamantanone I underwent ring cleavage by treatment with Ac2O and ClCO2R (R = Me, Et) to give diazabicylononanes II (R1 = CO2Me, CO2Et),

which were hydrolyzed to give II (R1 = H). Favorskii ethynylation of II (R1 = H, Me, Ac, PhCH2, Pr) gave the corresponding ethynyldiazabicyclononanols III. Piperidinones IV (R2 = Me, Pr; R3R4 = O) underwent Favorskii ethynylation and Grignard reaction with HC.tplbond.CMgBr gave epimeric piperidinols IV (R3, R4 = HO, HC.tplbond.C).

IT **15507-63-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 15507-63-8 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-oxo-1,5-diphenyl-, dimethyl ester (8CI, 9CI) (CA INDEX NAME)



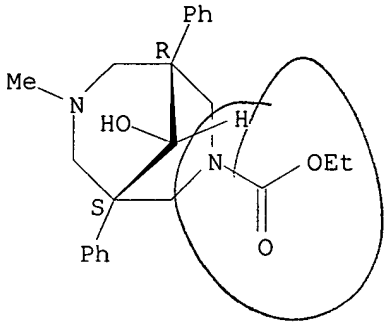
L7 ANSWER 11 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 92:163871 CA
TITLE: Relationship between basicity and molecular structure in polycyclic nitrogen compounds. II. Synthesis of the stereoisomeric monomethiodides of 3,7-dimethyl-1,5-diphenyl-9-bispidinol and of 1,3-diaza-5,7-diphenyl-6-adamantanol: influence of the hydroxy group on basicity
AUTHOR(S): Settimj, Guido; Del Giudice, Maria Rosaria; Di Simone, Luciano
CORPORATE SOURCE: Lab. Chim. Farm., Ist. Super. Sanita, Rome, 00161, Italy
SOURCE: Gazz. Chim. Ital. (**1979**), 109(6-7), 345-9
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The stereoisomeric monomethiodides of 3,7-dimethyl-1,5-diphenyl-9-bispidinol were prepd. from N-ethoxycarbonyl-N'-methyl-1,5-diphenyl-9-bispidinone through a 7-step synthesis and possess the expected difference of behavior to protonation. This difference of basicity is attributed to an intramol. interaction between the hydroxy group and the syn amino function, which is possible in only one of the two stereoisomers. The NMR, IR and pKa data of the intermediate asym. substituted derivs. of 9-bispidinol, belonging to the two stereoisomeric series, support the existence of such an intramol. interaction.

IT **73310-77-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

RN 73310-77-7 CA
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-7-methyl-1,5-diphenyl-, ethyl ester, anti- (9CI) (CA INDEX NAME)

Relative stereochemistry.



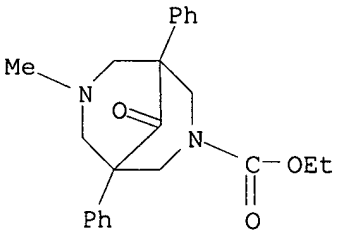
L7 ANSWER 12 OF 12 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 66:85777 CA
TITLE: Reactivity of 3,7-diazadamantanes. Synthesis of 1,5-diphenyl-3,7-diaza-10-thioadamantan-9-one 10-oxide and 10,-10-dioxide
AUTHOR(S): Misiti, Domenico; Chiavarelli, Stefano
CORPORATE SOURCE: Ist. Super. Sanita, Rome, Italy
SOURCE: Gazz. Med. Ital. (**1966**), 96(12), 1696-714
CODEN: GMITAB
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB (Tos = p-MeC6H4SO2Cl throughout this abstr.) To a cooled soln. of 3 g. I (X = CH2) (II) in 10 ml. anhyd. C5H5N, 1 ml. SO2Cl2 was added under stirring, the mixt. heated 0.5 hrs. at 40-50.degree., poured into H2O, the solid sepd. (3.5 g.) chromatographed on silica gel eluting with CHCl3, gave 1.4 g. I (X = SO2) (III), m. 246-7.degree.. Similarly, 3 g. II with 0.9 ml. SOCl2 in 10 ml. C5H5N kept 12 hrs. at room temp., then heated 0.5 hrs. at 40-50.degree., gave 0.62 g. I (X = SO) (IV), m. 183-4.degree.. The structures of III and IV were assigned on the basis of NMR spectra. Oxidn. of IV with Ca(MnO4)2 in 1:1 CHCl3-AcOH at -10.degree. gave III quant. II (0.02 mole) in 20 ml. C5H5N treated with 0.031 mole COCl2 in PhMe and the mixt. heated 7 hrs. at 80.degree. gave, instead of the expected I (X = CO), 1.45 g. of V (R = R' = COCl), m. 282-4.degree. (decompn.) (CHCl3-hexane). The same reaction, carried out in the absence of C5H5N gave V (R = COCl, R' = H) as HCl salt (not isolated), which dissolved in hot MeOH, the soln. treated with 0.1N NaOH and the sepd. solid chromatographed on silica gel eluting with CHCl3, led to V (R = CO2Me, R' = H) (VI), m. 133-5.degree.. Similarly, V (R = CO2Et, R' = H) (VII), m. 125-7.degree., was prepd. To confirm the structure, the known V (R = R' = CO2Et) (Chiavarelli and Settimj, CA 53, 22008a) was transformed by hydrolysis into a mixt. of VII and V (R = R' = H). Attempts to obtain I (X = CO) by heating VI, VII: a) 5 hrs. at 130.degree. without solvent, b) 10 hrs. in refluxing xylene, c) 5 hrs. in refluxing xylene and in the

presence of MeONa, failed. Equimol. amts. of II (6.08 g.) and TosCl in C5H5N kept overnight at room temp., then heated 5 hrs. at 50-60.degree. and the reaction products chromatographed by the usual procedure, gave 1.2 g. V (R = R' = Tos), m. 246-7.degree., and 0.54 g. V (R = Tos, R' = H), m. 169-70.degree.. Finally, II with ClCO2Me (molar ratio 1:0.5) in dioxane, refluxed 3 hrs., the pH of the mixt. adjusted to 8, the unreacted II filtered off after long standing of the mixt. at 0.degree., the filtrate evapd. and the residue chromatographed, gave in order the following V [R, R', and m.p. (CHCl3-hexane) given]: CO2Me, Me, 172-4.degree.; CO2Me, CO2Me, 192-4.degree.; CO2Me, CHO, 205-7.degree., VI. Similarly, equimol. amts. of II and ClCO2Et in CHCl3, refluxed 1 hr. and the reaction products chromatographed, gave in order the following V [R, R', and m.p. (EtOH) given]: CO2Et, Me, 151-2.degree.; CO2Et, CO2Et, 172-3.degree.; VII. The behavior of II with ClCO2R was discussed on the light of their cleavage products.

IT **7037-98-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and N.M.R. of)

RN 7037-98-1 CA

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-methyl-9-oxo-1,5-diphenyl-, ethyl ester (7CI, 8CI, 9CI) (CA INDEX NAME)



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L2 13 S L1
L3 199 S L2 FULL

FILE 'CA' ENTERED AT 14:01:31 ON 09 AUG 2001
L4 24 S L3
L5 13 S L4 AND PD < JULY 1999
L6 1 S L5 AND BJORSNE, M?/AU
L7 12 S L5 NOT L6

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=> s l3

L8 3 L3

=> d l8, all, 1-3

L8 ANSWER 1 OF 3 CAOLD COPYRIGHT 2001 ACS
AN CA65:8914b CAOLD
TI reactions with chloroacetaldehyde and 2,4-dichlorocrotonaldehyde
AU Kopp, Erwin; Smidt, J.
IT 105-39-5 105-48-6 107-20-0 274-76-0 1129-52-8 2929-73-9
3848-12-2 5409-75-6 6855-74-9 6855-92-1 6860-87-3
7038-01-9 **7038-02-0** 7038-05-3 7038-06-4
7038-07-5 7038-08-6 7038-09-7 7038-10-0 7038-11-1 7038-12-2
7038-14-4 7038-15-5 7038-16-6 7038-17-7 7038-18-8 7038-20-2
7038-23-5 7038-24-6 7038-25-7 7166-44-1 7166-45-2 7166-46-3
7166-48-5 7166-50-9 7166-51-0 7166-52-1 7166-53-2 7166-54-3
26394-31-0 89123-76-2 90153-90-5

L8 ANSWER 2 OF 3 CAOLD COPYRIGHT 2001 ACS
AN CA65:8913g CAOLD
TI synthesis of 1,5-diphenylbispidin-9-ones and-9-ols - (XI) synthesis of unsym. 1,5-diphenyl-3,7-dialkylbispidin-9-ones
AU Settimj, Guido; Landi-Vittory, R.; Gatta, F.; Sarti, N.; Chiavarelli, S.
IT 4208-18-8 4208-19-9 4398-13-4 4398-15-6 7037-92-5 7037-93-6
7037-94-7 **7037-98-1** **7037-99-2** **7038-00-8*****

L8 ANSWER 3 OF 3 CAOLD COPYRIGHT 2001 ACS
AN CA53:22008a CAOLD
TI 1,5-diphenyl-9-bispidinones and 1,5-diphenyl-9-bispidinols - (II) relation
between 1,5-diphenyl-9-bispidinone and -9-bispidinol and
1,5-diphenyl-3,7-diazaadamantan-9-one and -9-ol, (III)
3,7-dialkyl-1,5-diaryl-9-bispidinones and -9-bispidinols, (IV)
3,7-bis(aminoalkyl)- and (aminoacyl)-bispidones and bispidols
AU Chiavarelli, Stefano; Settimj, G.
IT 3576-75-8 4208-31-5 4208-32-6 ***13638-71-6 19066-35-4
23690-15-5 41432-71-7 57164-04-2 79168-88-0 79168-89-1 87703-07-9
87703-11-5 87864-73-1 102374-71-0 102660-32-2 102875-71-8 102889-39-4
102951-75-7 103161-47-3 103504-87-6 103504-96-7 103566-79-6 103566-80-9
103566-82-1 107150-01-6 107150-02-7 109046-21-1 109046-36-8 113751-59-0
113751-67-0 113861-18-0 113862-18-3 113862-19-4 113862-37-6 115000-34-5
115918-13-3 116029-67-5 116029-69-7 116029-70-0 117272-19-2 117272-20-5
118228-39-0

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.93	191.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.28

FILE 'REGISTRY' ENTERED AT 14:03:44 ON 09 AUG 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 8 AUG 2001 HIGHEST RN 350791-61-6
DICTIONARY FILE UPDATES: 8 AUG 2001 HIGHEST RN 350791-61-6

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT
for details.

=> e 7038-02-0/rn

E1	1	7038-00-8/RN
E2	1	7038-01-9/RN
E3	1 -->	7038-02-0/RN
E4	1	7038-05-3/RN
E5	1	7038-06-4/RN
E6	1	7038-07-5/RN
E7	1	7038-08-6/RN
E8	1	7038-09-7/RN

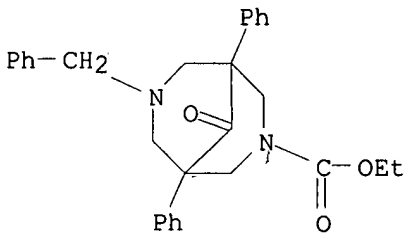
```
E9              1     7038-10-0/RN
E10             1     7038-11-1/RN
E11             1     7038-12-2/RN
E12             1     7038-14-4/RN

=> s e3

L9              1 7038-02-0/RN

=> d l9


L9   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2001 ACS
RN   7038-02-0  REGISTRY
CN   3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-benzyl-9-oxo-1,5-
     diphenyl-, ethyl ester (7CI, 8CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C29 H30 N2 O3
LC   STN Files:   BEILSTEIN*, CAOLD
         (*File contains numerically searchable property data)
```



102

```
                1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e  7038-01-9/rn

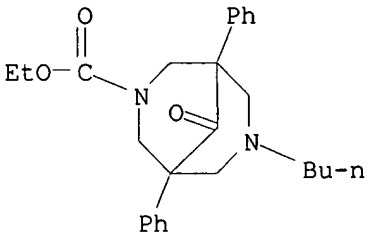
E1              1     70379-99-6/RN
E2              1     7038-00-8/RN
E3              1 --> 7038-01-9/RN
E4              1     7038-02-0/RN
E5              1     7038-05-3/RN
E6              1     7038-06-4/RN
E7              1     7038-07-5/RN
E8              1     7038-08-6/RN
E9              1     7038-09-7/RN
E10             1     7038-10-0/RN
E11             1     7038-11-1/RN
E12             1     7038-12-2/RN

=> s e3

L10             1 7038-01-9/RN

=> d l10
```

L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
RN **7038-01-9** REGISTRY
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-butyl-9-oxo-1,5-diphenyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H32 N2 O3
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e 7038-02-0/rn

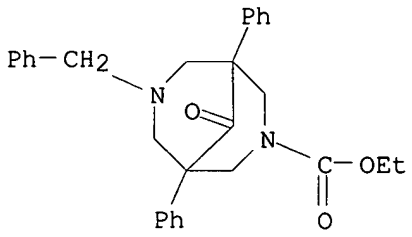
E1	1	7038-00-8/RN
E2	1	7038-01-9/RN
E3	1 -->	7038-02-0/RN
E4	1	7038-05-3/RN
E5	1	7038-06-4/RN
E6	1	7038-07-5/RN
E7	1	7038-08-6/RN
E8	1	7038-09-7/RN
E9	1	7038-10-0/RN
E10	1	7038-11-1/RN
E11	1	7038-12-2/RN
E12	1	7038-14-4/RN

=> s e3

L11 1 7038-02-0/RN

=> d l11

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
RN **7038-02-0** REGISTRY
CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-benzyl-9-oxo-1,5-diphenyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H30 N2 O3
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e 3576-75-8/rn

E1            1     3576-73-6/RN
E2            1     3576-74-7/RN
E3            1 --> 3576-75-8/RN
E4            1     3576-76-9/RN
E5            1     3576-77-0/RN
E6            1     3576-85-0/RN
E7            1     3576-86-1/RN
E8            1     3576-88-3/RN
E9            1     3576-92-9/RN
E10           1     3576-99-6/RN
E11           1     35760-00-0/RN
E12           1     35760-05-5/RN

=> s e3

L12           1 3576-75-8/RN

=> d l12


L12  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2001 ACS
RN   3576-75-8  REGISTRY
CN   1,3-Diazatricyclo[3.3.1.13,7]decan-6-ol, 5,7-diphenyl- (9CI)  (CA INDEX
     NAME)
OTHER CA INDEX NAMES:
CN   1,3-Diazaadamantan-6-ol, 5,7-diphenyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN   5,7-Diphenyl-1,3-diazaadamantan-6-ol
FS   3D CONCORD
MF   C20 H22 N2 O
CI   COM
LC   STN Files:   BEILSTEIN*, CA, CAOLD, CAPLUS, RTECS*, TOXLIT
         (*File contains numerically searchable property data)
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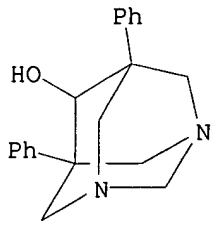


8 REFERENCES IN FILE CA (1967 TO DATE)
8 REFERENCES IN FILE CAPLUS (1967 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e 4208-31-5/rn

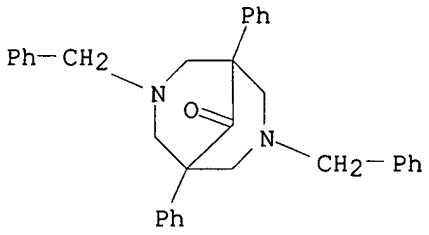
E1	1	4208-27-9/RN
E2	1	4208-30-4/RN
E3	1 -->	4208-31-5/RN
E4	1	4208-32-6/RN
E5	1	4208-33-7/RN
E6	1	4208-34-8/RN
E7	1	4208-35-9/RN
E8	1	4208-40-6/RN
E9	1	4208-41-7/RN
E10	1	4208-42-8/RN
E11	1	4208-45-1/RN
E12	1	4208-46-2/RN

=> s e3

L13 1 4208-31-5/RN

=> d l13

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
RN **4208-31-5** REGISTRY
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-diphenyl-3,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dibenzyl-1,5-diphenyl- (6CI, 7CI, 8CI)
FS 3D CONCORD
MF C33 H32 N2 O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS
(*File contains numerically searchable property data)



8 REFERENCES IN FILE CA (1967 TO DATE)
8 REFERENCES IN FILE CAPLUS (1967 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e 4208-32-6/rn

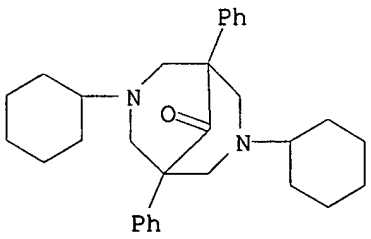
E1            1     4208-30-4/RN
E2            1     4208-31-5/RN
E3            1 --> 4208-32-6/RN
E4            1     4208-33-7/RN
E5            1     4208-34-8/RN
E6            1     4208-35-9/RN
E7            1     4208-40-6/RN
E8            1     4208-41-7/RN
E9            1     4208-42-8/RN
E10           1     4208-45-1/RN
E11           1     4208-46-2/RN
E12           1     4208-47-3/RN

=> s e3

L14           1 4208-32-6/RN

=> d l14

L14  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2001 ACS
RN   4208-32-6  REGISTRY
CN   3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclohexyl-1,5-diphenyl- (6CI,
     7CI, 8CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C31 H40 N2 O
LC   STN Files:   BEILSTEIN*, CAOLD, CHEMCATS
         (*File contains numerically searchable property data)
```



2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e 13638-71-6/rn

E1            1     13638-68-1/RN
E2            1     13638-69-2/RN
E3            1 --> 13638-71-6/RN
E4            1     13638-72-7/RN
E5            1     13638-73-8/RN
E6            1     13638-74-9/RN
E7            1     13638-75-0/RN
E8            1     13638-76-1/RN
E9            1     13638-77-2/RN
E10           1     13638-78-3/RN
E11           1     13638-79-4/RN
E12           1     13638-80-7/RN

=> s e3

L15           1 13638-71-6/RN

=> d l15

L15  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2001 ACS
RN   13638-71-6  REGISTRY
CN   3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-oxo-1,5-diphenyl-,
     diethyl ester (6CI, 8CI, 9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C25 H28 N2 O5
LC   STN Files:   BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT
         (*File contains numerically searchable property data)
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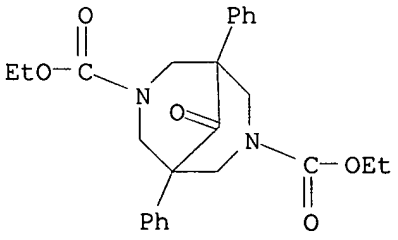

5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> d his

     (FILE 'HOME' ENTERED AT 14:00:48 ON 09 AUG 2001)

     FILE 'REGISTRY' ENTERED AT 14:00:52 ON 09 AUG 2001
```

```
L1              STRUCTURE UPLOADED
L2           13 S L1
L3          199 S L2 FULL

     FILE 'CA' ENTERED AT 14:01:31 ON 09 AUG 2001
L4           24 S L3
L5           13 S L4 AND PD < JULY 1999
L6            1 S L5 AND BJORSNE, M?/AU
L7           12 S L5 NOT L6

     FILE 'CAOLD' ENTERED AT 14:03:24 ON 09 AUG 2001
L8            3 S L3

     FILE 'REGISTRY' ENTERED AT 14:03:44 ON 09 AUG 2001
                E   7038-02-0/RN
L9            1 S E3
                E  7038-01-9/RN
L10           1 S E3
                E  7038-02-0/RN
L11           1 S E3
                E 3576-75-8/RN
L12           1 S E3
                E  4208-31-5/RN
L13           1 S E3
                E 4208-32-6/RN
L14           1 S E3
                E 13638-71-6/RN
L15           1 S E3

=>

---Logging off of STN---


=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    12.05     203.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -7.28

STN INTERNATIONAL LOGOFF AT 14:06:50 ON 09 AUG 2001
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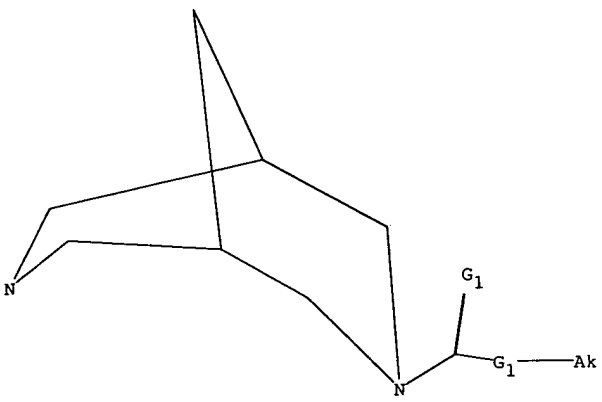
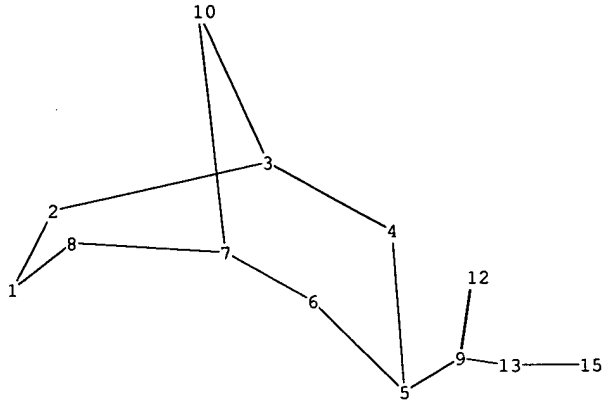
STN Structure : 09623705.str



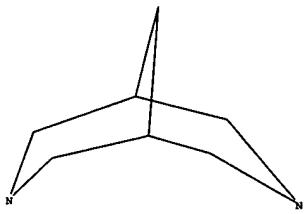


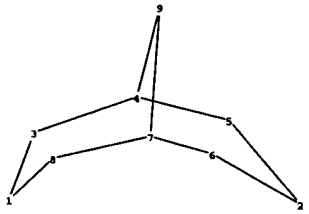
chain nodes :
9 12 13 15
ring nodes :
1 2 3 4 5 6 7 8 10
chain bonds :
5-9 9-12 9-13 13-15
ring bonds :
1-2 1-8 2-3 3-4 3-10 4-5 5-6 6-7 7-8 7-10
exact/norm bonds :
1-2 1-8 2-3 3-4 3-10 4-5 5-6 5-9 6-7 7-8 7-10 9-12 9-13 13-15
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
12:CLASS 13:CLASS 15:CLASS

C:\stnweb\Queries\705a.str

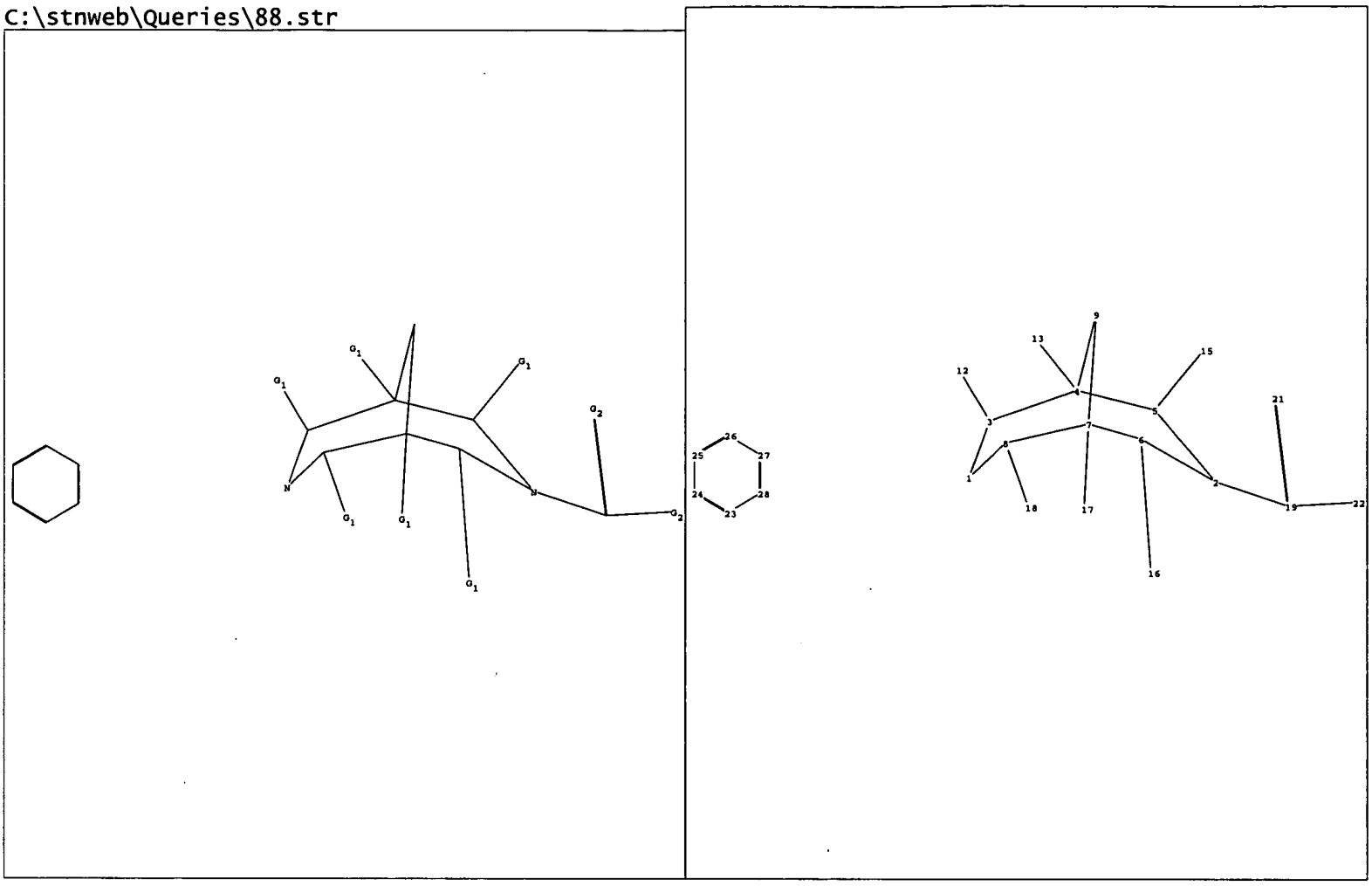




ring nodes :
    1 2 3 4 5 6 7 8 9
ring bonds :
    1-3 1-8 2-5 2-6 3-4 4-5 4-9 6-7 7-8 7-9
exact/norm bonds :
    1-3 1-8 2-5 2-6 3-4 4-5 4-9 6-7 7-8 7-9
isolated ring systems :
    containing 1 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

C:\stnweb\Queries\88.str



chain nodes :
12 13 15 16 17 18 19 21 22
ring nodes :
1 2 3 4 5 6 7 8 9 23 24 25 26 27 28
chain bonds :
2-19 3-12 4-13 5-15 6-16 7-17 8-18 19-21 19-22
ring bonds :
1-3 1-8 2-5 2-6 3-4 4-5 4-9 6-7 7-8 7-9 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
1-3 1-8 2-5 2-6 2-19 3-4 3-12 4-5 4-9 4-13 5-15 6-7 6-16 7-8 7-9 7-17 8-18
19-21 19-22
normalized bonds :
23-24 23-28 24-25 25-26 26-27 27-28
isolated ring systems :
containing 1 : 23 :

G1:Ak,H

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:CLASS 13:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom